Supplementary information

Valorization of waste coffee grounds into microporous carbon materials for CO_2 adsorption

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Adsorption Kinetics study

Adsorption kinetics, cyclic stability, and facile regeneration are equally important factors for high CO_2 adsorption capacity. To evaluate the adsorption kinetics, here we have measured time-dependent CO_2 adsorption isotherms of CAC3 using TGA at various temperatures 303, 313, and 323 K under atmospheric pressure (see manuscript). The experimental data were fitted by pseudo-first-order and pseudo-second-order models. Both models explain adsorption rate where pseudo-first-order depends upon the number of adsorption sites (**Eq. S1**) while pseudo-second-order assumes the square of the number of adsorption sites (**Eq. S2**).

$$q_t = q_e\left(1 - e^{-k_1 t}\right) \qquad (S1)$$

$$q_t = \frac{1}{\frac{1}{k_2 q_e^2 t} + \frac{1}{q_e}} \qquad (S2)$$

here, q_e and q_t denote adsorption uptakes at equilibrium and time "t", respectively. Additionally, k_1 and k_2 denote adsorption rate constants obtained by fitting the experimental data, with pseudo-first and pseudo-second order, respectively. Notably, pseudo-first-order best fits the experimental data with R^2>0.99 at all temperatures, compared to pseudo second-order, which further indicate the physical adsorption mechanism of CO_2 capture [1, 2]. Additionally, the activation energy was also determined using the following **Eq. S3**.

$$k_1 = A\exp\left(-\frac{E_a}{RT}\right) \qquad (S3)$$

here "A" is Arrhenius' exponential factor, "E_a" is the activation energy, "R" is the universal gas constant, and "T" represents absolute temperature. A linear fitting graph between the natural log of k_1 and inverse of temperature (*i.e.*, 1/T) was drawn (see manuscript). The activation energy based on obtained fitted parameters was calculated to be 5.36 kJ mol^{-1}, revealing the CO_2 adsorption mechanism predominantly physisorption [3].

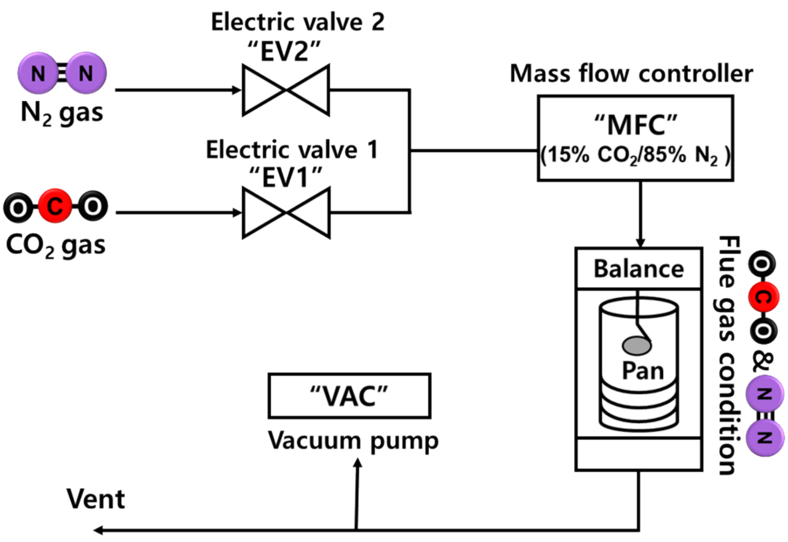

Fig. S1. Experimental setup of the binary mixture gas adsorption (gravimetric analysis) and cycling measurements

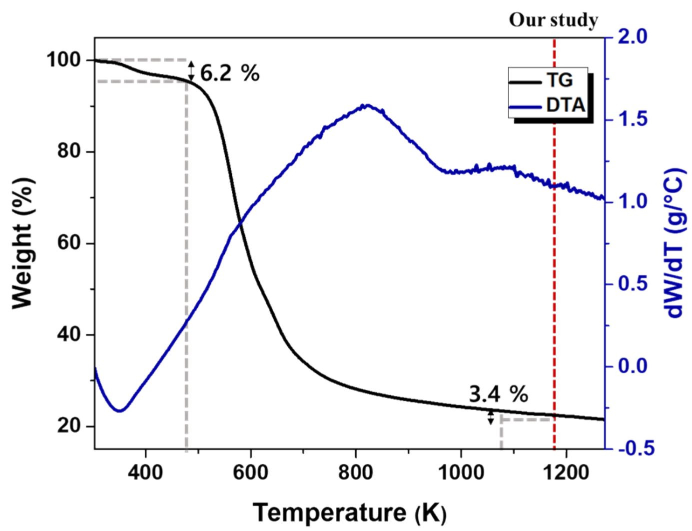

Fig. S2. TG-DTA curve for coffee grounds under nitrogen atmosphere

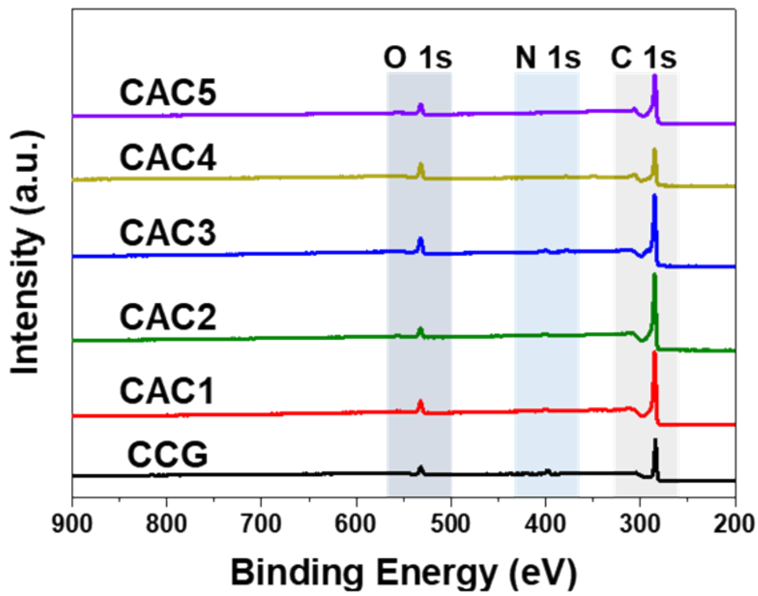

Fig. S3 XPS survey scan for all samples.

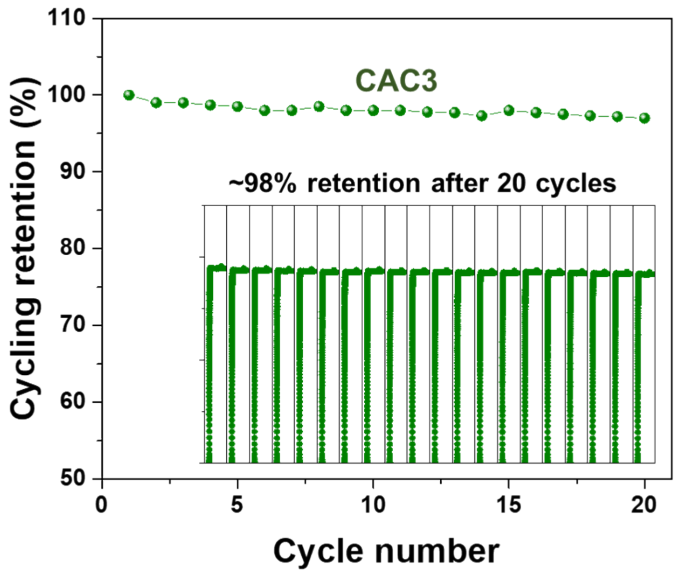

Fig. S4 Flue gas condition 20 cycle retention

Table S1. The initial isosteric heat of CO_2 adsorption of CCG and CAC samples.

Samples	Initial isosteric heat of adsorption (kJ/mol)
CAC1	27.4
CAC2	30.6
CAC3	34.4
CAC4	30.0
CAC5	25.6

Table S2. Comparisons of biomass-derived activated carbons and their performance in CO_2 uptakes

Samples	Biomass Precursor	Activating agents	Activation conditions		Specific surface area (m^2 g^{-1})	CO_2 uptakes at 273 K/1 bar (mmol g^{-1})	References
			Temp. (K)	Time (h)			
CAC3	Coffee waste	$K_2C_2O_4$	1173	1	1714	6.91	This work
SM10 $K_2C_2O_4$	Sucrose/ Melamine	$K_2C_2O_4$	1073	1	3318	6.0	[4]
STO	Corn starch	$K_2C_2O_4$	1073	2	1747	6.12	[5]
300-6-K_2CO_3	Pecan nutshell	K_2CO_3	648	6	842	3.3	[6]
H250-800	Lotus stalk	KOH	1073	2	2510	3.42	[7]
K3-PDC1	Bee pollen	KOH	1073	2	1460	3.71	[8]
CPC-CA-SE/ACs	Pine cone	KOH	873	1	1786	6.57	[9]

Table. S3 The kinetic parameters for CAC3 samples based on CO_2 adsorption data fitting using psuedo first-order and pseudo second-order models at 303, 313, and 323 K.

Samples	Temperature (K)	Psuedo first-order		Psuedo second-order	
		K_1 (min^{-1})	R^2	K_2 ($mmol\ g^{-1}\ min^{-1}$)	R^2
CAC3	303	1.59	0.99624	2.06	0.88603
	313	1.71	0.99132	2.39	0.86849
	323	1.81	0.99712	3.02	0.90115

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